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Final Report DURIP Equipment Award, AFOSR #F49620-94-1-0460

This equipment award was used to purchase high-end computer workstations that have been used to enhance the research conducted under the parent award AFOSR #F49620-95-10198 and the associated AFOSR AASERT award #F49620-93-1-0323. Both strictly computational and high-end visualization equipment was obtained. On the computational side a share of a 40 CPU parallel work-station farm of DEC alpha machines was purchased. The workstation farm is located on campus in the University of Maryland Institute for Advanced Computer Studies (UMIACS) building. As provided by a large NSF infrastructure award to campus, access from my own computer laboratory to the remote super-computer farm facility is via a high-speed (ATM) fiber optic connection. An ATM switch to link all of the workstations in the local lab, is to be installed in the next few weeks. One of the machines to be integrated in this way is the graphics workstation purchased under the DURIP award. That purchase was only made in the last several months. It is a two processor Silicon Graphics Onyx with Infinite Reality Graphics. This is the highest performance graphics currently available from any manufacturer in the world at any price, and was purchased using DURIP funds at a deep academic discount (43%). With the local graphics capabilities and the high speed networking to the CPU farm, we have established a world class high performance computing facility.

The particular equipment purchased was tailored to further my groups research in interactive computation involving path following and multi-parameter continuation, with the computation being steered by the user who monitors the computation in real time using advanced visualization techniques applied to the ensuing bifurcation diagrams. On the software side we are currently integrating and extending the capabilities of two prior codes developed in the lab, namely MC^2 (Multiplier and Constraint Continuation), which was designed to implement interactive multi-parameter continuation on comparatively small problems, and PCR, which is a visualization and data-compression post-processor for the one-parameter continuation code AUTO. The outcome will be a single code with graphics implemented in OpenGL and Motif, that will allow interactive steering of multi-parameter numerical continuation computations of the solution set of systems of nonlinear two-point boundary value problems, with the visualization running on the local graphics machine, and the computation running on remote high-performance facilities. Because of the speed requirements imposed by interactivity, and the number of individual computations required for multi-parameter continuation such computations have only been made feasible with the hardware provided through the DURIP award. The primary application area within which we are developing our software and computational techniques is the continuum modelling of varioous macro-molecules. The research on this application is in collaboration with the Materials Lab at WPAFB and is partially supported through an Air Force Phase II SBIR from Wright Labs.